

铁苋菜中的一个新化合物

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摘要 从云南省富民县产铁苋菜(*Acalypha australis* L.)全草中分离并鉴定了一个新化合物, 命名为铁苋菜素(australisin)。通过光谱分析测定了其结构。此外, 还分离到 β -谷甾醇(β -sitosterol)和胡萝卜甾(daucosterol)。

关键词 铁苋菜, 大戟科, 铁苋菜素

A NEW COMPOUND FROM ACALYPHA AUSTRALIS

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Abstract A new compound named australisin (1) was isolated from the whole herb of *Acalypha australis* L. (Euphorbiaceae). Its structure was established by a spectroscopic analysis. In addition, β -sitosterol and daucosterol were also obtained.

Key words *Acalypha australis*, Euphorbiaceae, Australisin

INTRODUCTION

Acalypha australis L. (Euphorbiaceae), annual herb, usually occurs as a troublesome weed in farmlands and road sides throughout the southern China. The whole herb is used in the treatment of dysentery, diarrhea, abdominal distension, expectorant, uterus hemorrhage, dermatitis, and eczema^[1,2]. Earlier work on the genus *Acalypha* showed the presences of alkaloid, amide, glucoside and sterol.^[3,4]

We studied the chemical constituents of the whole herb of *Acalypha australis* L. collected in Fuming County, Yunnan Province, China in September, 1990. A new compound was isolated and named australisin (1). Its structure was determined by spectroscopic analysis.

RESULTS AND DISCUSSION

Australisin (1) showed the presences of three methoxy groups($\text{CH}_3\text{O} \times 3$), three methine groups (C-3,4,7), five quarternary carbons(C-5,6,8,9,10), two olefinic carbons(C-1', C-2') and four ketonic carbons(C-1, -COO- $\times 3$) in the ^1H NMR and ^{13}C NMR(DEPT) spectra of (1) (Table 1). The IR absorptions were indicated of the presences of benzene ring($1600\text{--}1518\text{cm}^{-1}$), hydroxyl(3400cm^{-1}), and olefinic group(1615cm^{-1}). The $^1\text{H}\text{--}^{13}\text{C}$ COSY spectrum of (1) showed the correlation signal between the C-2'(δ 129.7) and H-2'(δ 7.12), C-7 (δ 108.9) and H-7 (δ 7.88), C-4 (δ 35.6) and H-4(δ 6.21), C-3

(δ 79.4) and H-3(δ 5.88) and three correlation signals between the carbon and the hydrogen in each carboxymethyl group, respectively. In the ^1H - ^1H COSY spectrum of (1), the coupling correlation signal between H-3 (δ 5.88) and H-4 (δ 6.21) with a small coupling constant ($J = 1.6$ Hz), H-4 (δ 6.21) and H-2' (δ 7.12) could be observed, and the connection of C-3 and C-4 was determined. Therefore, we suggested that australisin possessed a carbon skeleton similar to chebulic acid (2) ^[5].

Table 1 ^1H NMR and ^{13}C NMR data of australisin(1)(400 MHz, $\text{C}_5\text{D}_5\text{N}$, TMS)

C	δ_{C} (ppm)	δ_{H} (ppm)	C	δ_{C} (ppm)	δ_{H} (ppm)
1	164.7s		1'	143.3s	
3	79.4d	5.88(1H,d,J = 1.6Hz)	2'	129.7d	7.12(1H, br s)
4	35.6d	6.21(1H,br s)	COOCH ₃	170.7s	
5	117.8s			52.9q	3.50(3H, s)
6	141.5s			166.9s	
7	108.9d	7.88(1H, s)		52.5q	3.50(3H, s)
8	147.6s			166.0s	
9	116.5s			52.1q	3.65(3H, s)
10	145.3s				

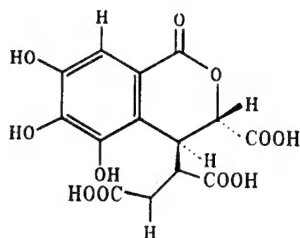
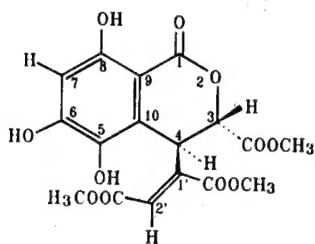
Assignments were based on ^1H - ^{13}C COSY.

Fig.1: australisin(1)

chebulic acid(2)

In order to determining the location of the aromatic proton, the COLOC spectrum of (1) was measured. It was the long-range correlation signals of (1) from its COLOC spectrum in Table 2. Therefore, the aromatic proton was located at the C-7 position.

Table 2 Long-range correlation signals from COLOC of australisin
(C₅D₅N, 400 MHz, TMS)

H	C-1	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-1'	C-2'	-COO- (166.0)	-COO- (166.9)	-COO- (170.7)
3	*		*					*		*				*
4		*		*				*	*	*	*		*	*
7	*			*	*		*	*						
2'			*								*		*	
-OCH ₃ (3.65)												*		
-OCH ₃ (3.50)													*	
-OCH ₃ (3.50)														*

The unusual lowfield chemical shift for H-4(δ 6.21) was caused by two weak hydrogen bonding effect between COOCH₃-3 and H-4, and COOCH₃-1' and H-4 (Fig. 2).

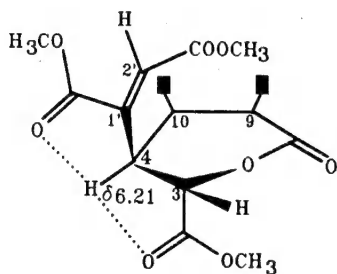


Fig.2: Hydrogen bonds within australisin(1)

Long-range coupling pattern between H-4 and H-2' was observed in the ¹H-¹H COSY spectrum of (1), and the configuration of the double bond was a trans one. Thus, the structure of australisin is (1).

EXPERIMENTAL SECTION

Mps: uncorr.; IR: KBr; ¹H NMR (400.13MHz) and ¹³C NMR (100.52 MHz), TMS as int. standard; EI-MS: 70eV.

Extraction and isolation: The air-dried whole plant (1300g) were powdered and ex-

tracted with MeOH (50°C). Evapn. of the solvent afford a residue (118g), which was descoloured by active charcoal and dissolved in H₂O. The aq. solution was extracted with EtOAc. The lipophilic phase (34g) was chromatographed over silica gel, eluted with the increasing proportions of PE-EtOAc. In the PE-EtOAc (3:7) elution, australisin (0.05g) was obtained and finally purified by recrystallization.

Australisin(1), C₁₇H₁₆O₁₁, ([M]⁺m/z396), colorless crystal. mp: 151—153.5°C. IR ν_{\max}^{KBr} cm⁻¹: 3400, 2950, 1725, 1615, 1600, 1518, 1485, 1430, 1375, 1300—1225, 1110, 1050. EIMS m/z (70eV): 396 [M]⁺, 305 (base). ¹H NMR and ¹³C NMR data see Table 1.

β -Sitosterol, colorless needles. mp 140°C. IR ν_{\max}^{KBr} cm⁻¹: 3500, 2930, 1470, 1380, 1065, 960. MS m/z: 414, 396, 381, 329, 303, 273, 255, 213, 43. Mp, IR, TLC were identical with an authentic sample.

Daucosterol, amorphous powder. mp > 300°C. IR ν_{\max}^{KBr} cm⁻¹: 3400, 2960, 2930, 2850, 1450, 1375, 1360, 1160, 1100, 1075, 1025. IR and TLC were identical with an authentic sample.

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